Lecture on

Semiconductors / 半導体

(Physics of semiconductors)

2021.4.7 Lecture 01

Institute for Solid State Physics, University of Tokyo

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How the lecture will go on?

- Powerpoint (converted to pdf) file will be uploaded in the corresponding ITC-LMS site, (https://itc-lms.ecc.u-tokyo.ac.jp/lms/course?idnumber=202135603-00290F01) by the day before the lecture.
- The lecture notes (in Japanese, English) will be uploaded in the site https://kats.issp.u-tokyo.ac.jp/kats/semicon4/ by the end of the lecture week.
- Small amount of problems for your exercise at home will be given in the last of the lecture in every two weeks. Submission deadline of the solutions is two weeks later. I hope I can collect them through LTC-LMS but if that is difficult I will prepare my own web script.
- In the very last of the lecture in July, the problems for your report will be given. The deadline for the submission of the report will be notified then.
- The lecture is recorded on the cloud. I hope I can upload the video for one or two weeks.
- I hope I can find some ways to get questions from you (via chat, etc.?)

Lecture Plan

Related site: https://kats.issp.u-tokyo.ac.jp/kats/semicon4/

1) Crystal structure and crystal growth
2) Energy band, effective mass approximation
3) Carrier statistics and chemical doping
4) Optical properties
5) Semi-classical treatment of charier transport
6) Homo/hetero junctions, semiconductor devices (optical, electrical)
7) Quantum structures (quantum wells, wires, dots) by nanofabrication techniques
8) Basics of quantum transport
9) Galvanomagnetic effects, Quantum Hall effects
10) Spin-related phenomena (spintronics)
11) Topological effects

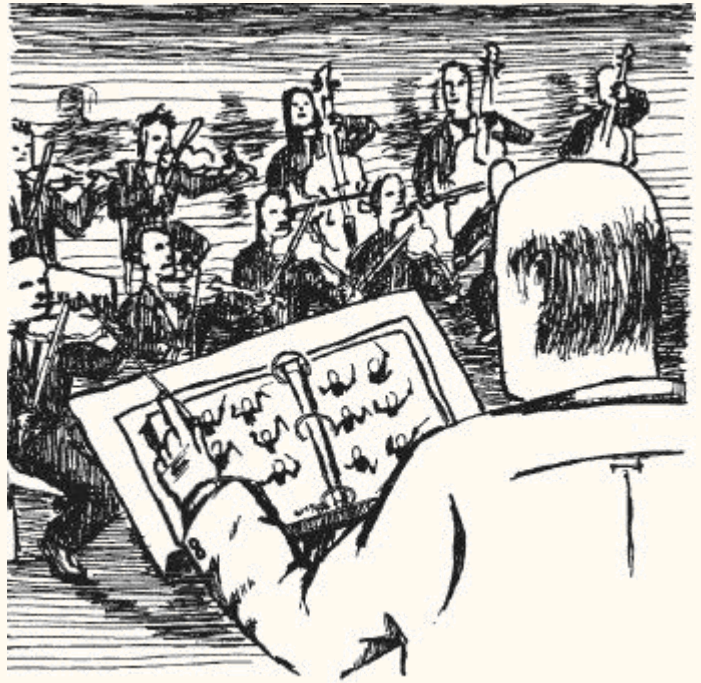
１）結晶構造と結晶成長
２）エネルギーバンド，有効質量モデル
３）半導体キャリア統計とドーピング
４）光学的性質
５）電気伝導の半古典論
６）ホモ・ヘテロ接合，半導体デバイス（光，電子）
７）微細構造技術による量子構造（量子井戸，細線，ドット）
８）量子輸送の基礎
９）電流磁気効果，量子ホール効果
１０）スピン物性 (スピントロニクス)
１１）トポロジカル効果

Characteristics of semiconductors

- Not metal
- Middle range band gap
- Weak divergence of resistivity with lowering temperature

Structure sensitive (conduction) properties

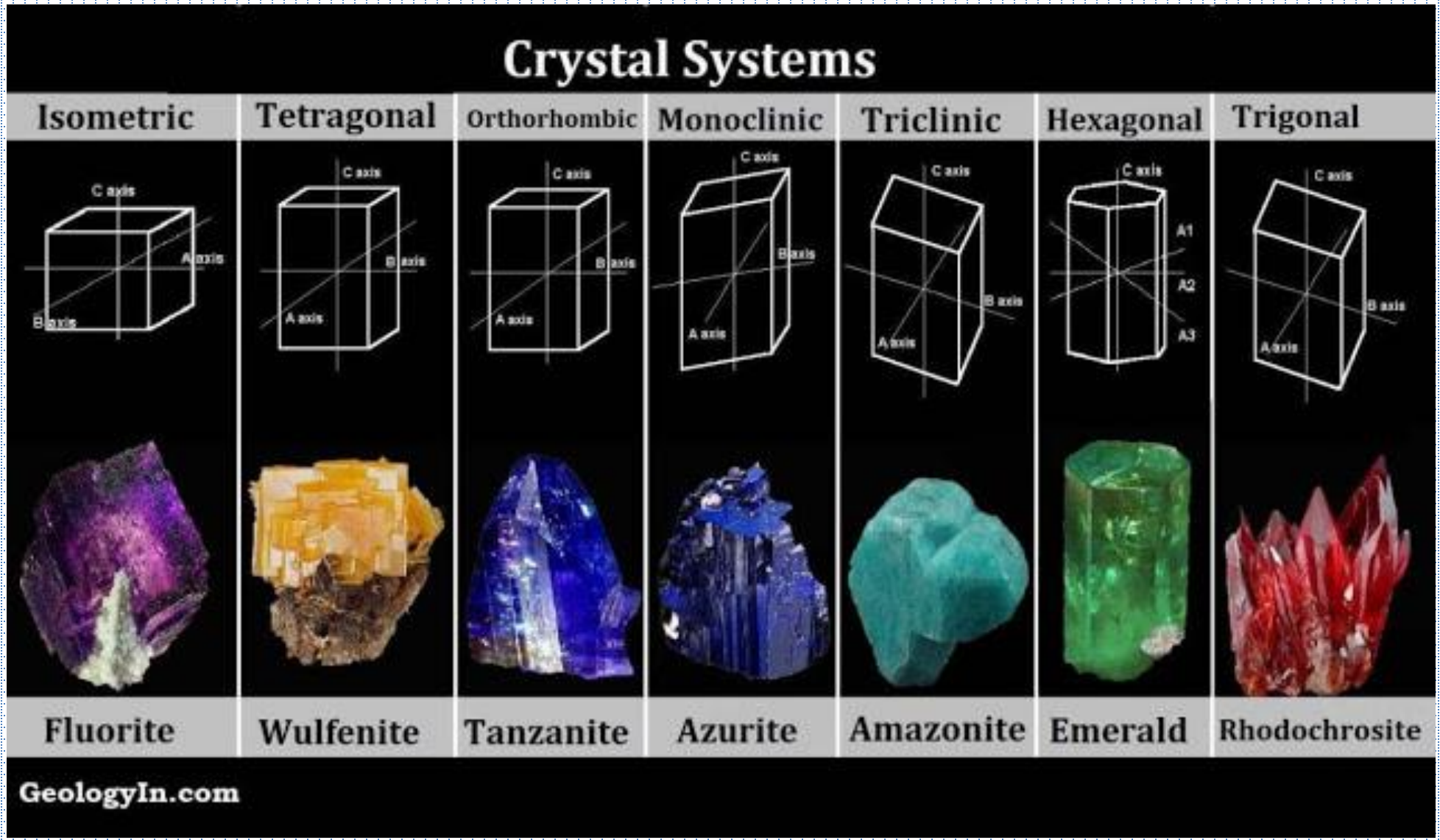
- Drastic changes in electric conduction with ultra-small amount of impurities
- Changes in electronic and optical properties with quantum confinement structures like quantum wells, wires, and dots



A SEMI-CONDUCTOR

Yu & Cardona, "Fundamentals of Semiconductors"

Chapter 1 Crystal structures and crystal growths



http://www.geologyin.com/2014/11/crystal-structure-and-crystal-system.html

Crystal structure

Uniform solids
- crystals
  - poly
  - single
- amorphous

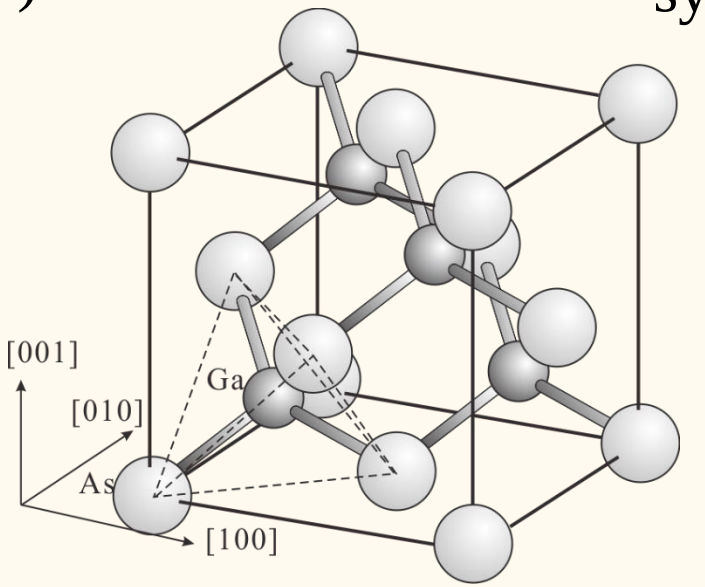
Crystals: Spatially periodic structures

Unit of spatial repetition

Primitive cell: unit of spatial repetition with smallest number of atoms

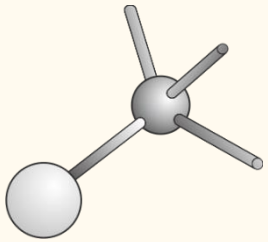
Unit cell: unit of spatial repetition taken as for human to find symmetry of the crystal

ex) GaAs



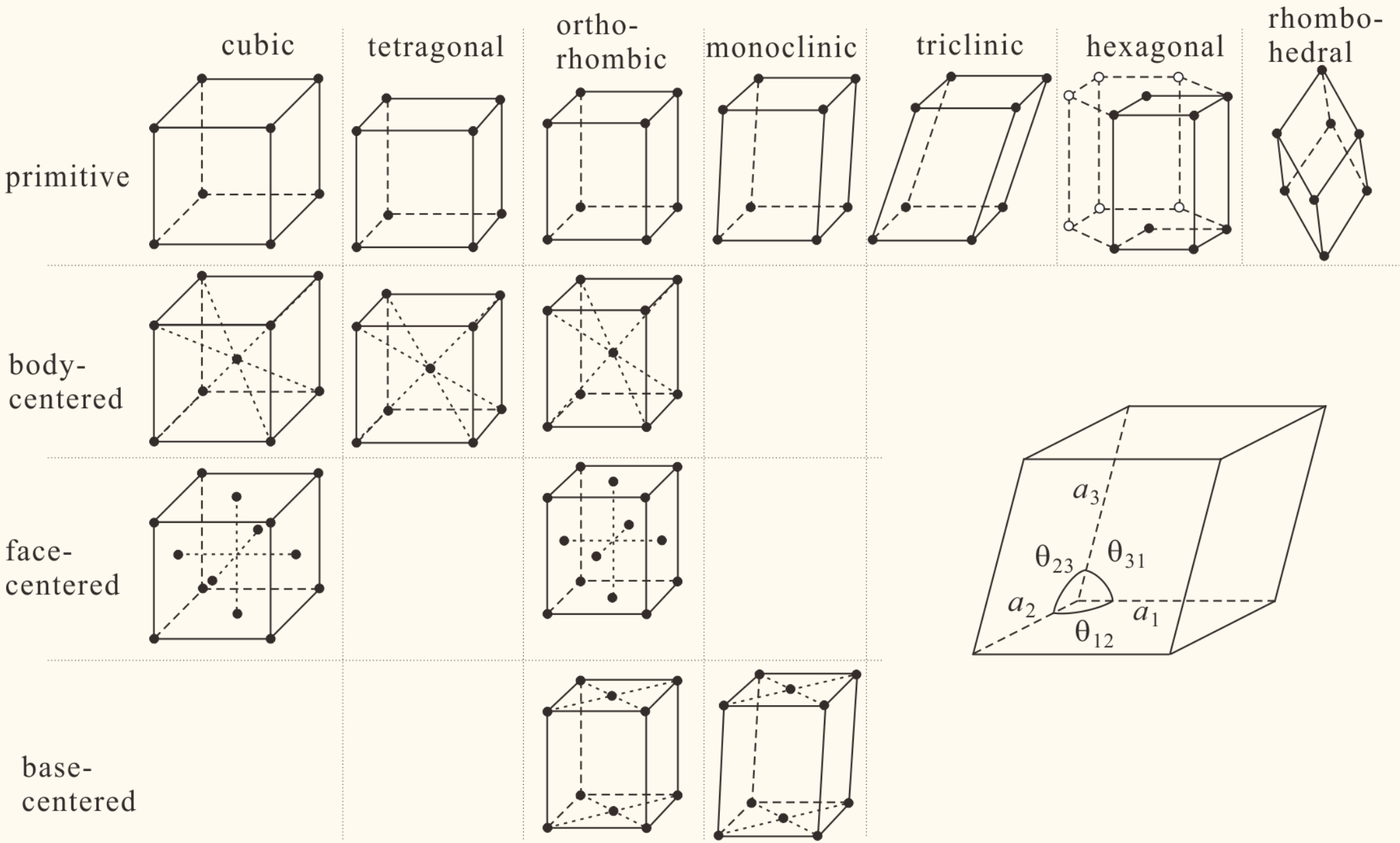
Unit cell

face centered cubic (fcc)



Primitive cell

Bravais lattices



Lattice, reciprocal lattice (1)

Lattice: spatial repetition of the unit structure.

$$\boldsymbol{r}' = \boldsymbol{r} + \sum_{i=1,2,3} l_i \boldsymbol{a}_i = \boldsymbol{r} + \boldsymbol{R}$$

l_i: integers, $\boldsymbol{a}_i$: primitive (translation) vector

$\boldsymbol{R}$: lattice vector

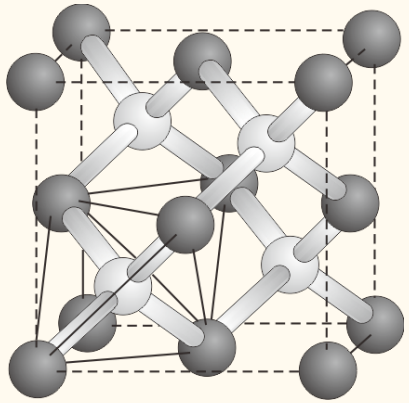
Lattice potential $U(\boldsymbol{r})$ $\quad U(\boldsymbol{r}) = \sum_{\boldsymbol{G}} U_{\boldsymbol{G}} e^{i\boldsymbol{G}\boldsymbol{r}}$

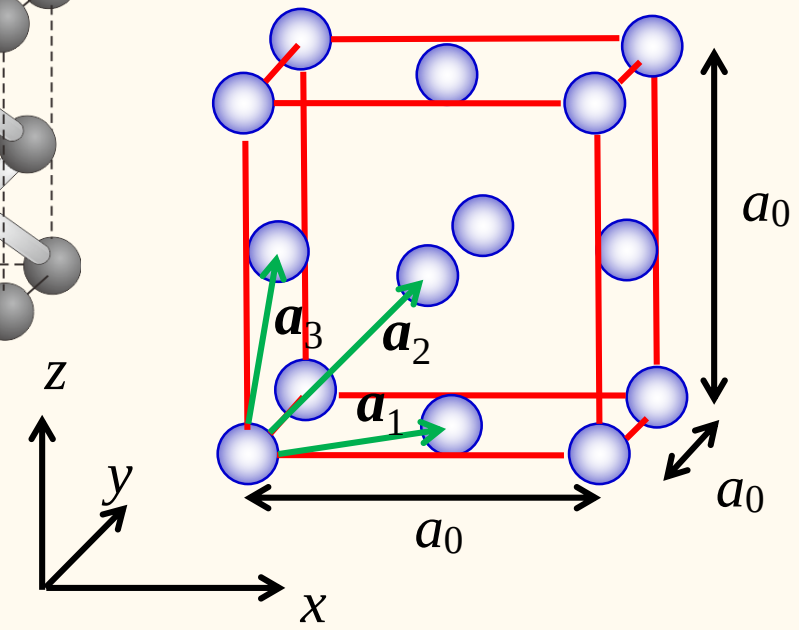
$$U(\boldsymbol{r} + \boldsymbol{R}) = U(\boldsymbol{r})$$

$$\boldsymbol{G} \cdot \boldsymbol{R} = 2\pi n \quad (n : \text{integer}), \quad \therefore e^{i\boldsymbol{G}\cdot\boldsymbol{R}} = 1$$

$\boldsymbol{G}$: reciprocal lattice vector

ex) diamond structure (fcc)





$$\boldsymbol{a}_1 = \frac{a_0}{2}(\boldsymbol{e}_x + \boldsymbol{e}_y), \quad \boldsymbol{a}_2 = \frac{a_0}{2}(\boldsymbol{e}_y + \boldsymbol{e}_z),$$
$$\boldsymbol{a}_3 = \frac{a_0}{2}(\boldsymbol{e}_z + \boldsymbol{e}_x)$$

Lattice, reciprocal lattice (2)

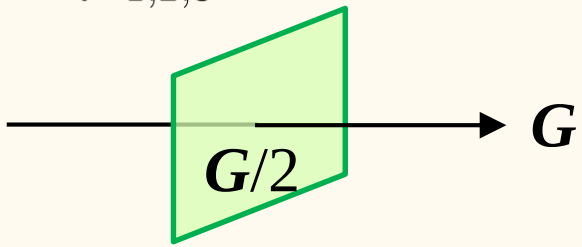
$$|A| \equiv \boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$$

$$\boldsymbol{b}_1 = \frac{2\pi \boldsymbol{a}_2 \times \boldsymbol{a}_3}{|A|}, \quad \boldsymbol{b}_2 = \frac{2\pi \boldsymbol{a}_3 \times \boldsymbol{a}_1}{|A|},$$

$$\boldsymbol{b}_3 = \frac{2\pi \boldsymbol{a}_1 \times \boldsymbol{a}_2}{|A|}$$

primitive reciprocal vectors

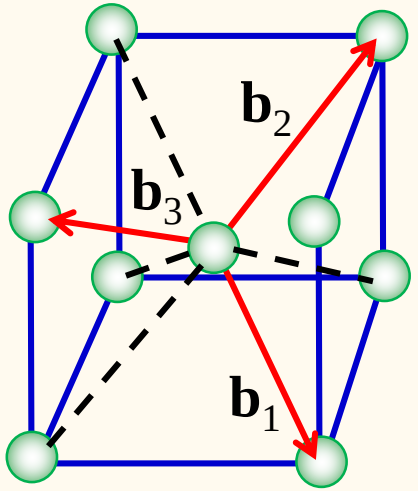
$$\boldsymbol{G} = \sum_{i=1,2,3} h_i \boldsymbol{b}_1, \quad (h_i: \text{integer})$$



Plane that cuts $\boldsymbol{G}$ at $\boldsymbol{G}/2$ vertically

→ unit cell in the reciprocal lattice:

Brillouin zone



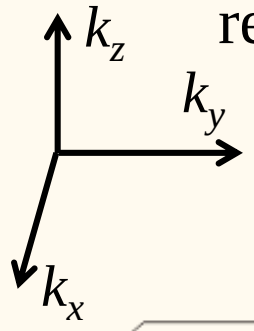
First Brillouin zone

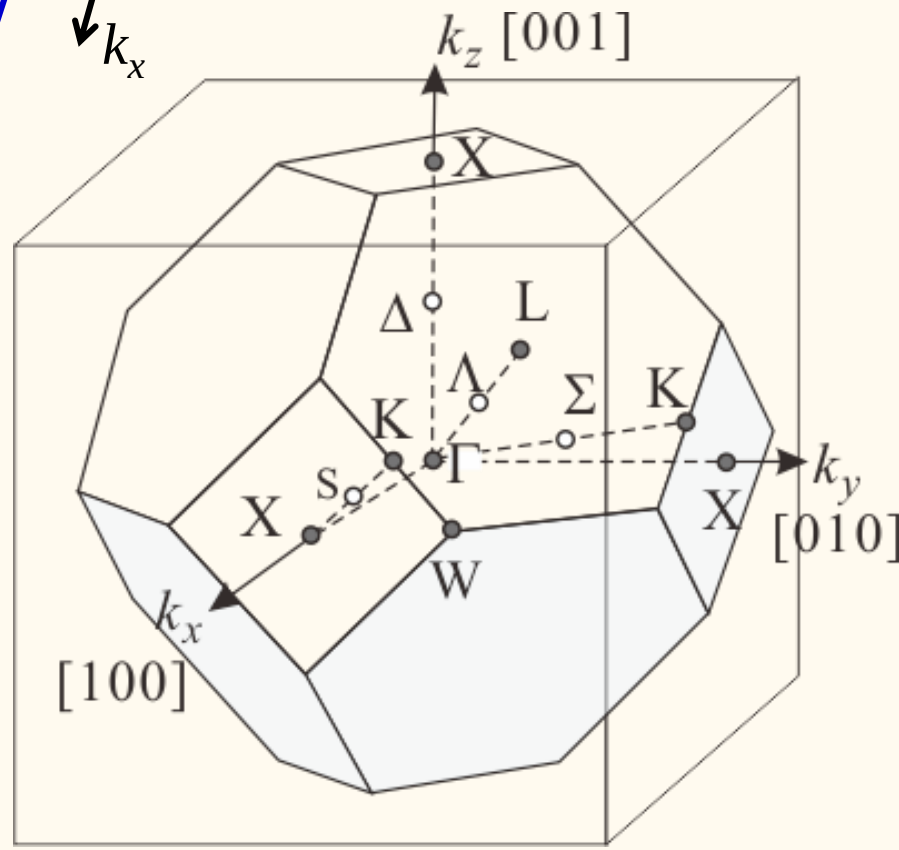
Points with high symmetries:

Γ, X, L, W

ex) diamond structure (fcc)

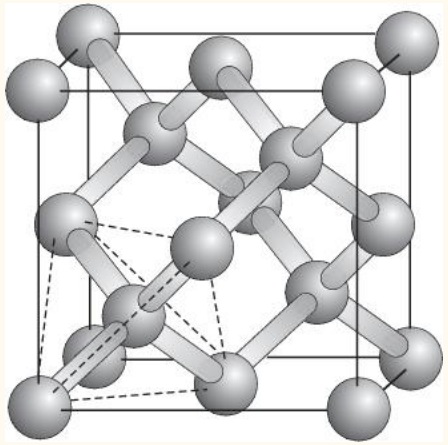
reciprocal lattice: bcc





Inorganic crystals often used as semiconductors: Group IV

Diamond structure (fcc)



diamond

silicon

germanium

II	III	IV	V	VI
4 Be ベリリウム 9.012182	5 B ホウ素 10.811	6 C 炭素 12.0107	7 N 窒素 14.0067	8 O 酸素 15.9994
12 Mg マグネシウム 24.305	13 Al アルミニウム 26.98153...	14 Si ケイ素 28.0855	15 P リン 30.973762	16 S 硫黄 32.065
30 Zn 亜鉛 65.38	31 Ga ガリウム 69.723	32 Ge ゲルマニウム 72.63	33 As ヒ素 74.9216	34 Se セレン 78.96
48 Cd カドミウム 112.411	49 In インジウム 114.818	50 Sn スズ 118.71	51 Sb アンチモン 121.76	52 Te テルル 127.6

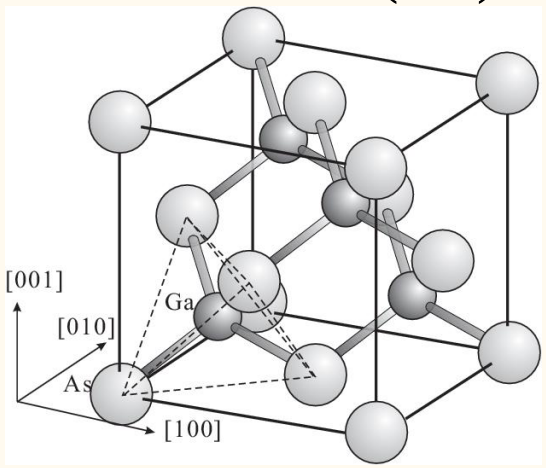
(α-Sn)

SiC

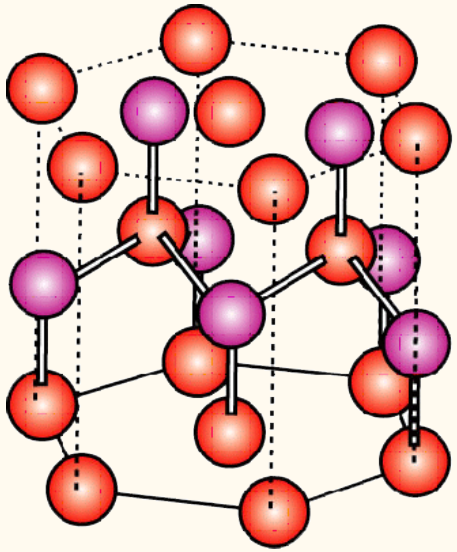
Si_xGe_{1-x}

Inorganic crystals often used as semiconductors: Group III-V

Zinc-blende (fcc)



Wurzeit (hexagonal)

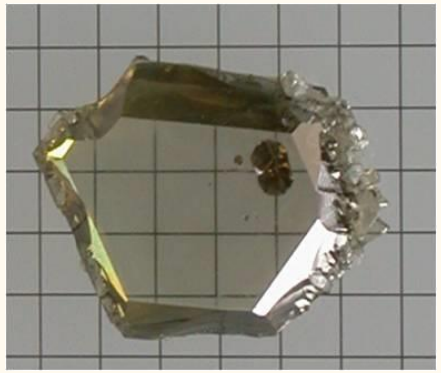


GaAs

(ZB)

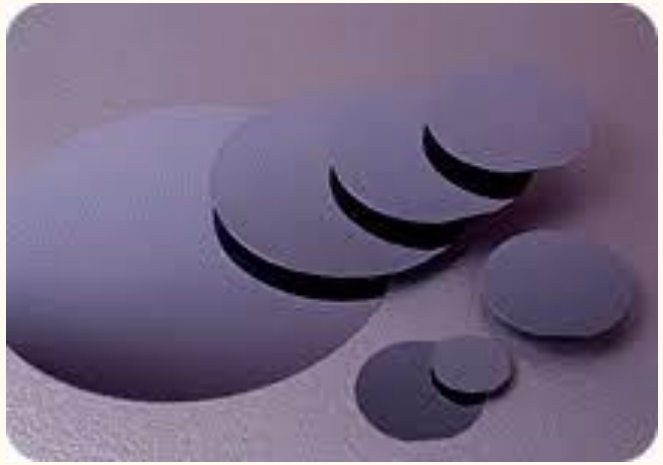
GaN

(WZ)



CdTe

(ZB)



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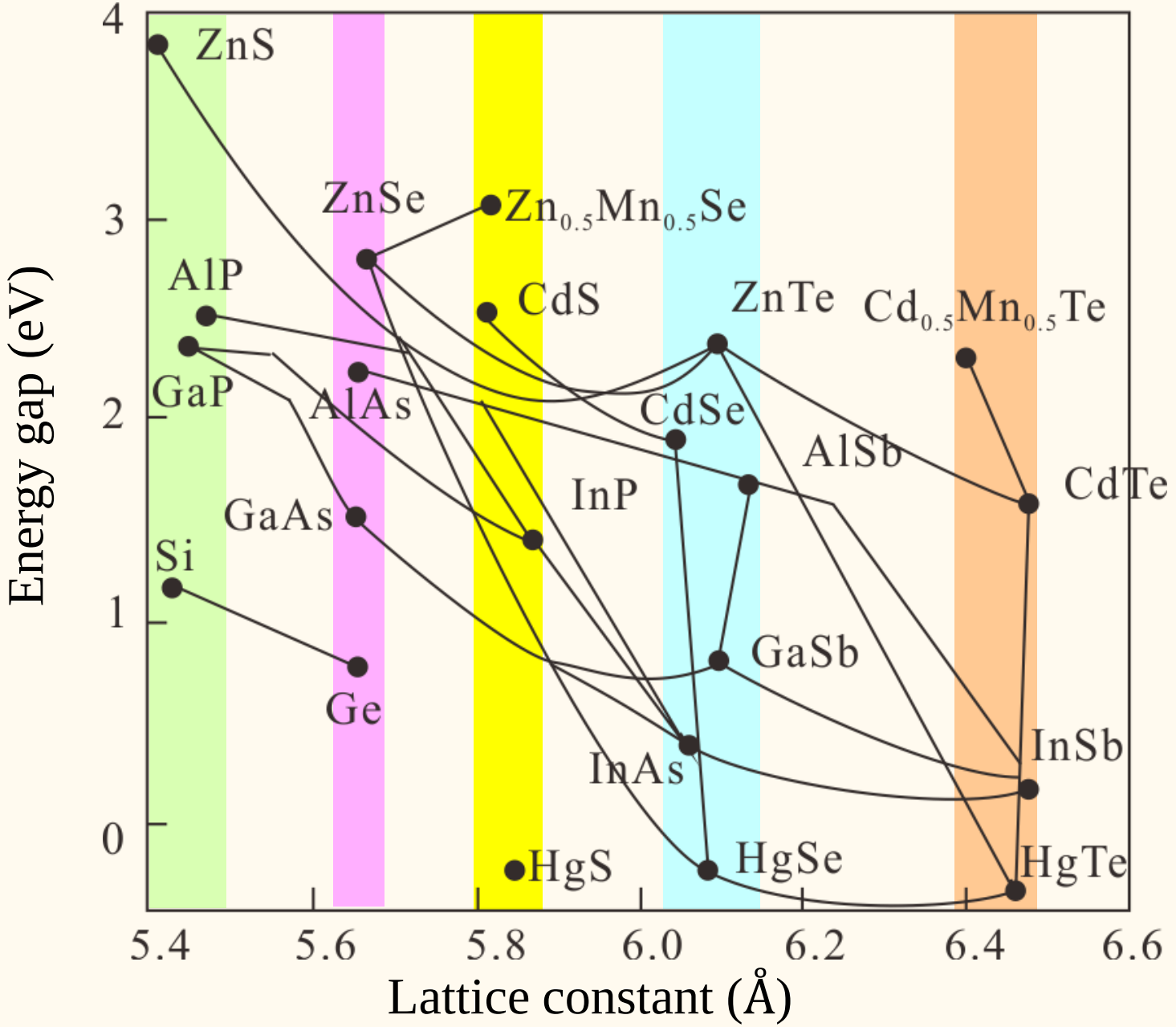
Energy gaps and lattice constants of representative (cubic) semiconductors



Room temperature

Colored stripes:
Lattice matching groups
→ Heterojunctions are available

Lines: Mixed crystals

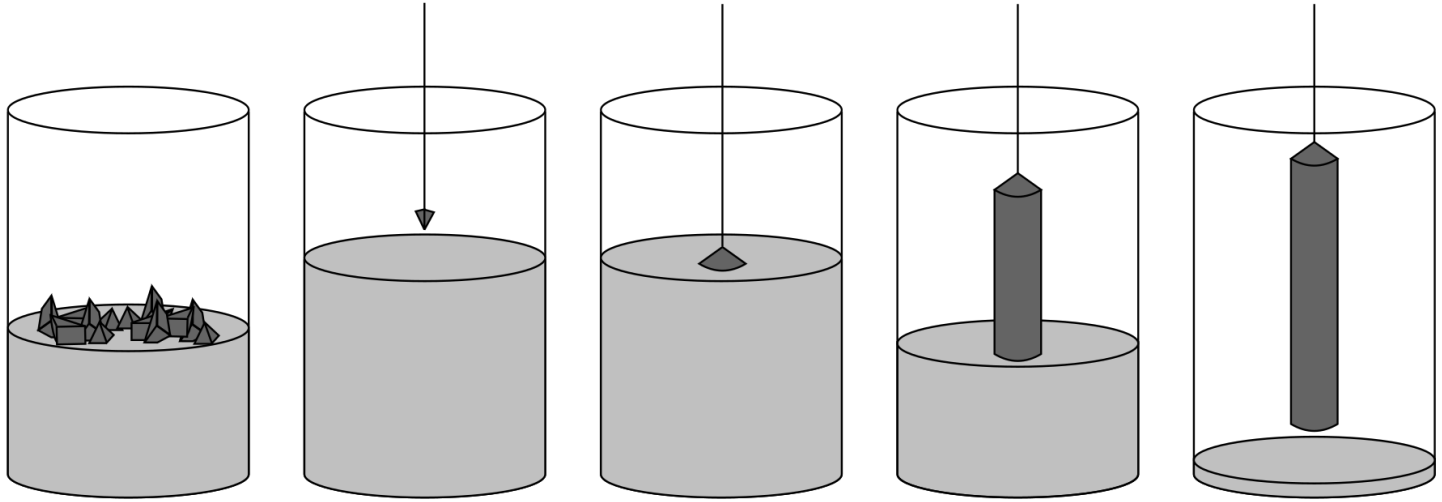
GaN (Wurzeit)
a = 3.19 Å, c = 5.19 Å
3.4 eV (RT)

Various methods for semiconductor crystal growth

- Bulk growth
  - Vertical
    - Czochralski
    - Bridgman
    - Floating zone melting
  - Horizontal
    - Horizontal Bridgman
    - Zone melting
- Thin film growth
  - Chemical Vapor Deposition (Vapor Phase Epitaxy)
    - Thermal decomposition
      - chloride
      - organic metal
    - Plasma
  - Liquid Phase Epitaxy
  - Molecular Beam Epitaxy
  - Atomic Layer Deposition
  - Laser ablation

"Tree-like" classification is actually difficult.

Crystal growth: Czochralski method



Melting of polysilicon, doping

Introduction of the seed crystal

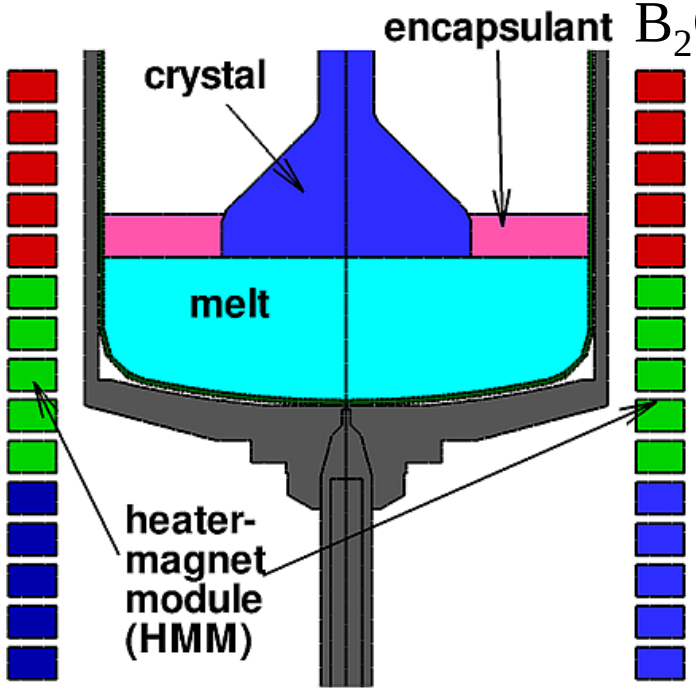
Beginning of the crystal growth

Crystal pulling

Formed crystal with a residue of melted silicon

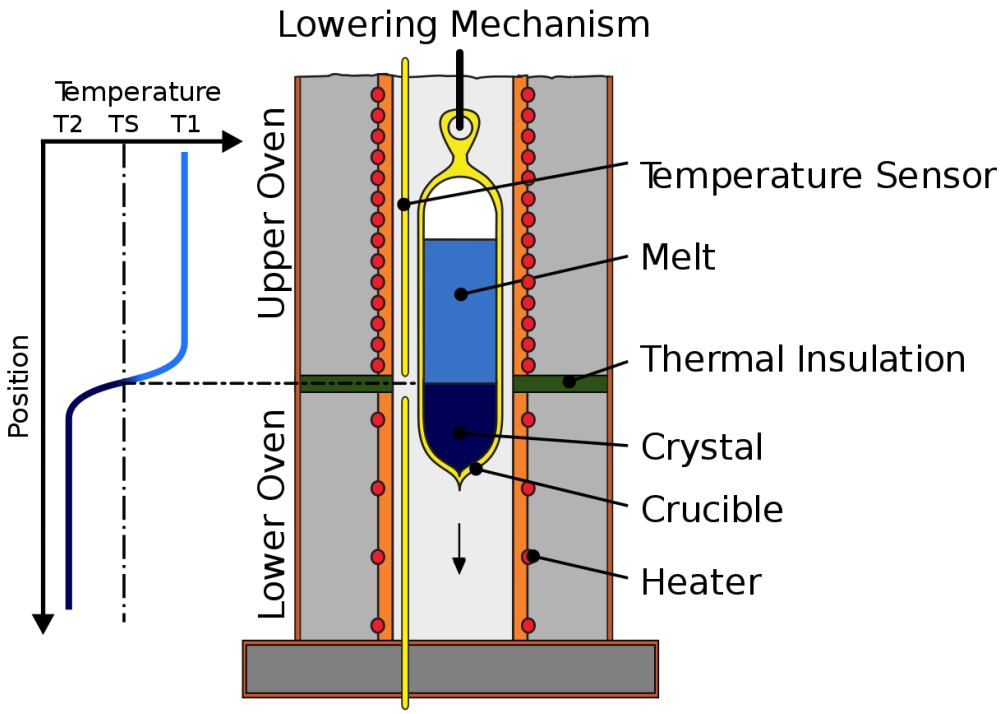
Czochralski method for silicon (Wikipedia)

Liquid encapsulated Czochralski (LEC) (GaAs, InP, etc. high vapor pressure materials)



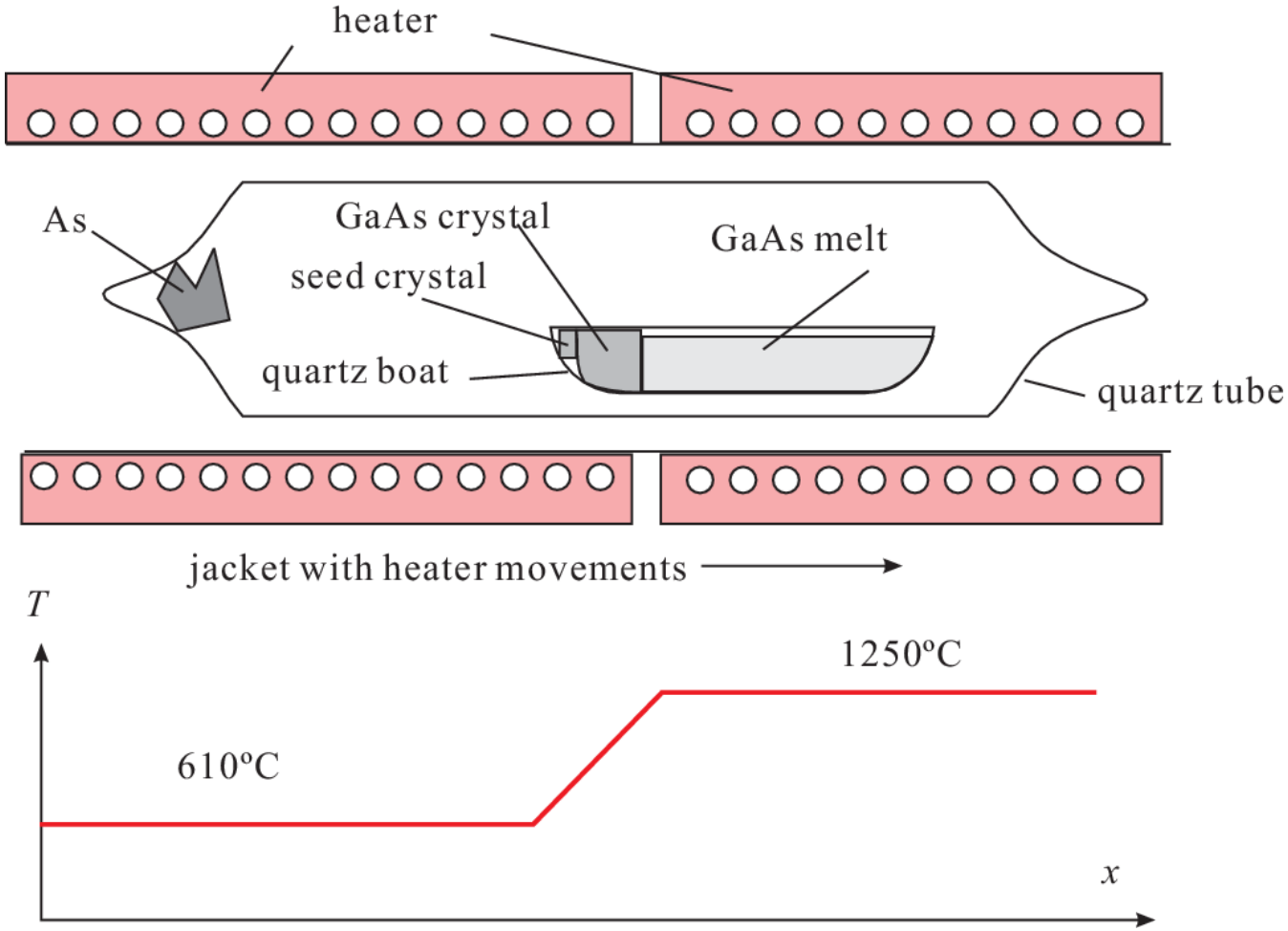
Bridgman methods

Bridgman-Stockbarger method



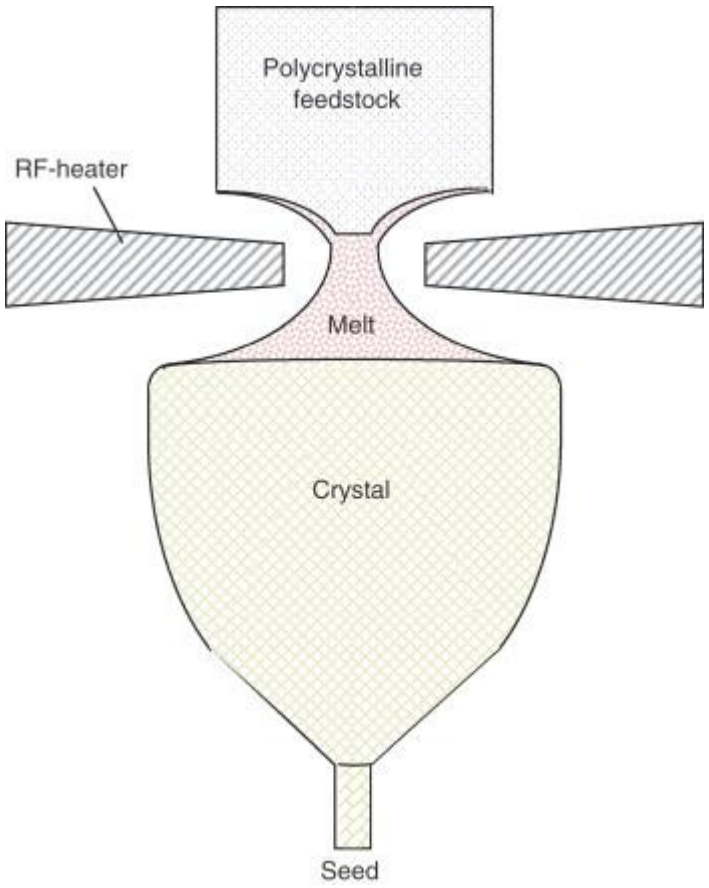
From Wikipedia

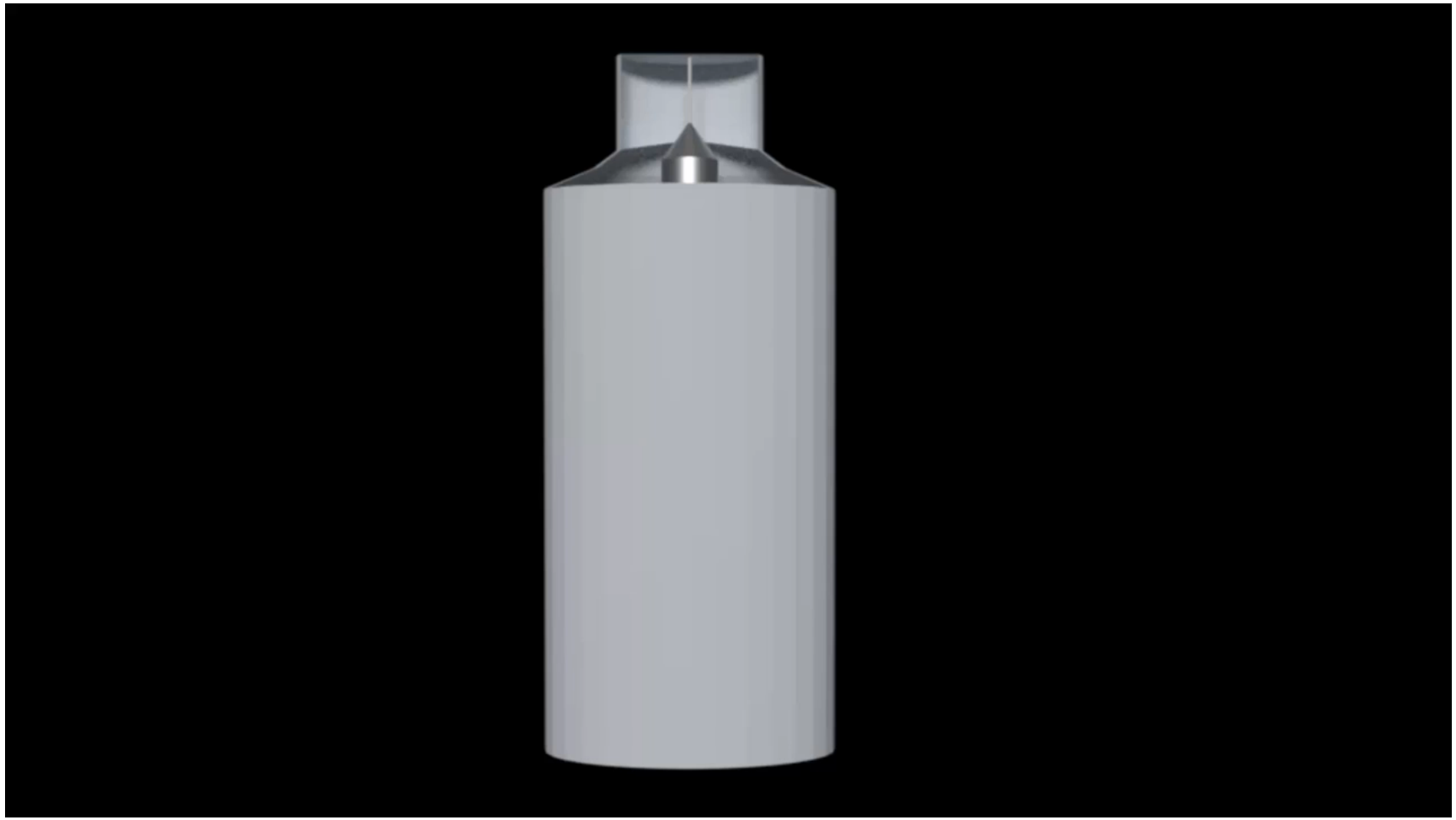
Horizontal Bridgeman (HB) process



temperature gradient freezing method

Floating zone method

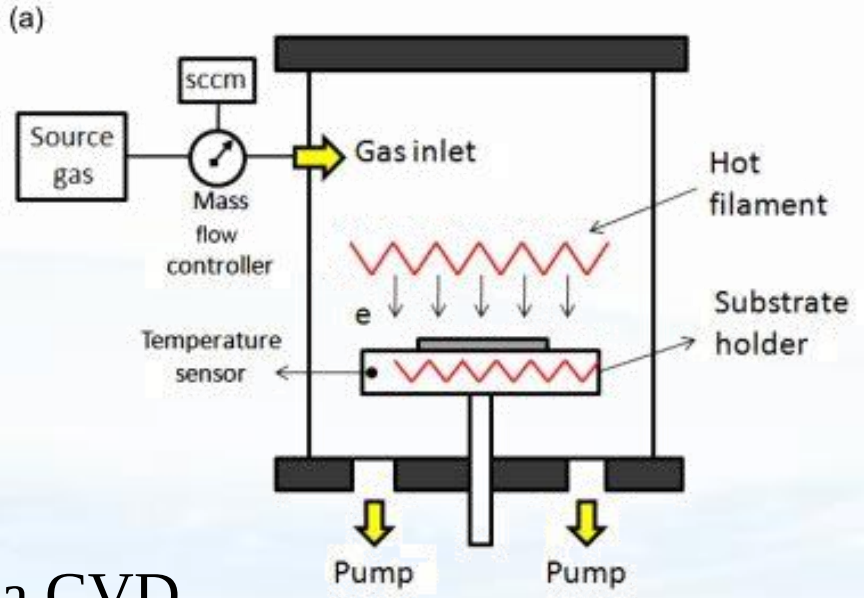




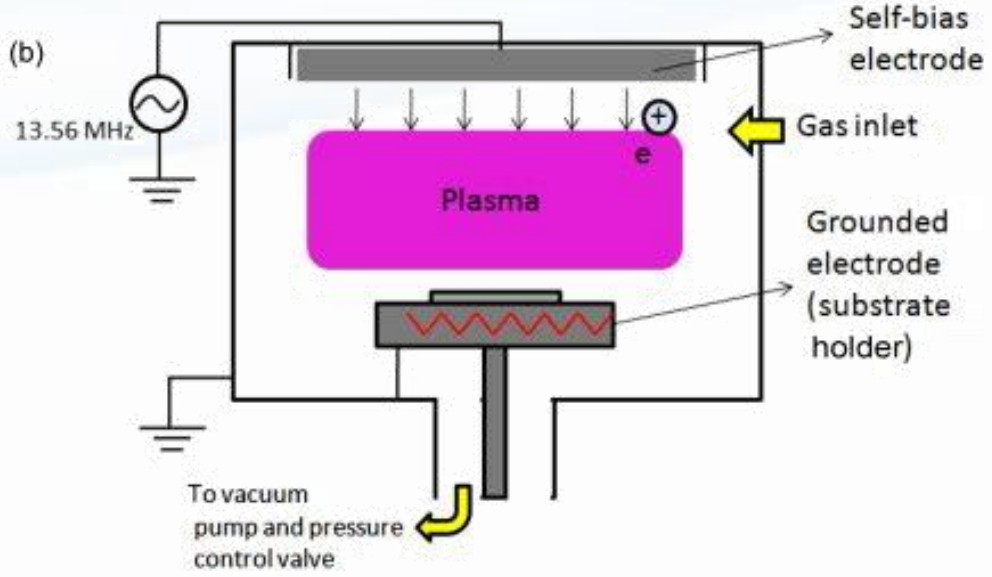
https://www.youtube.com/watch?v=jPijg8NIamo

Chemical vapor deposition (CVD), metal-organic CVD (MOCVD)

Thermal decomposition

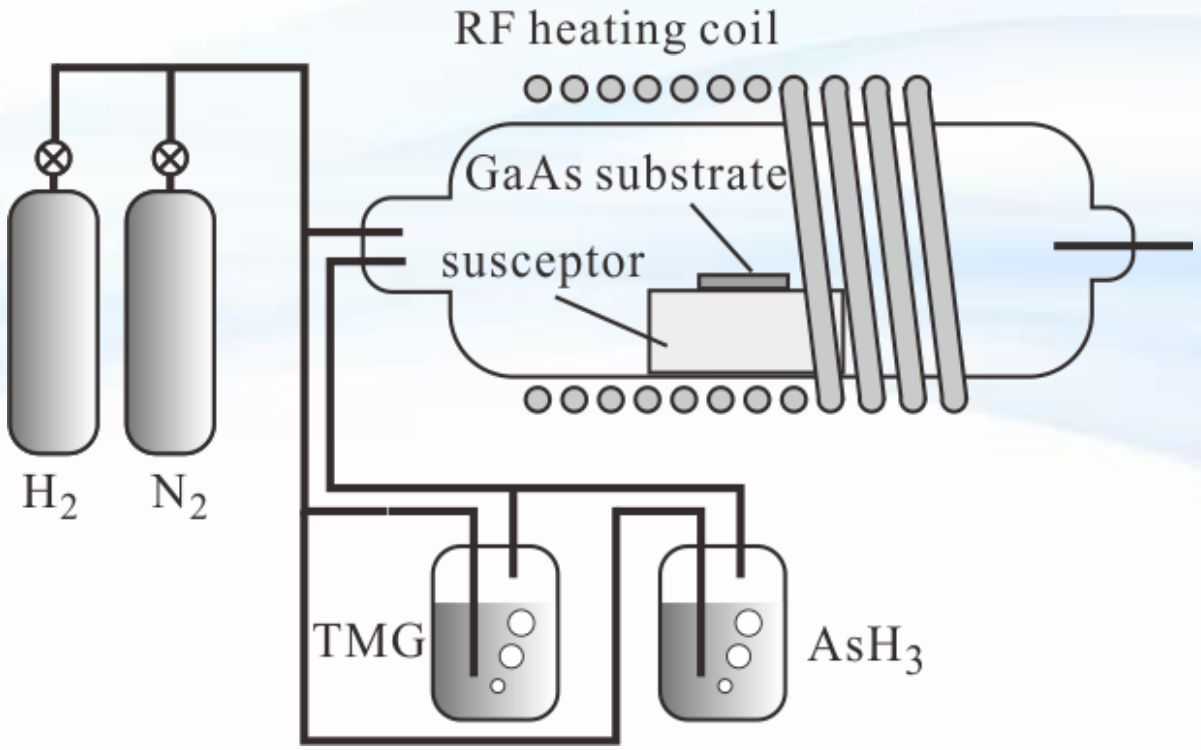


Plasma CVD



MOCVD

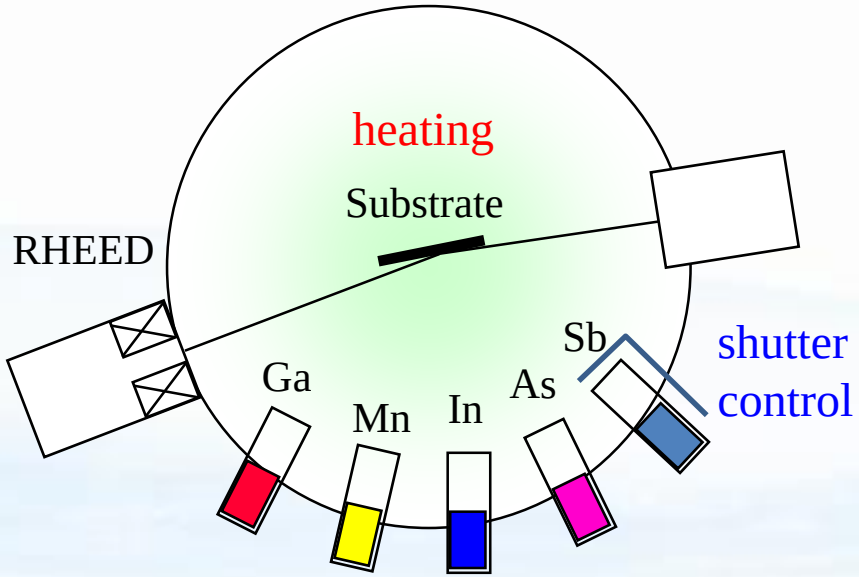
(organometallic vapor phase epitaxy, OMVPE)



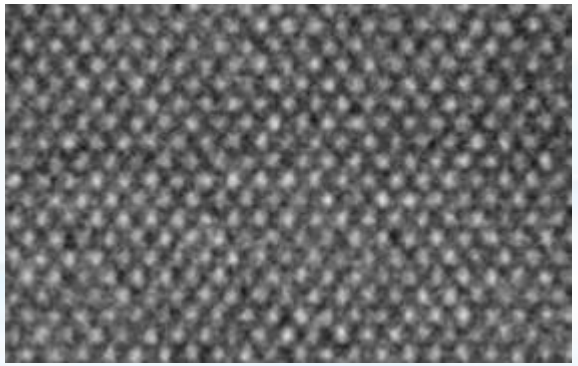
Organic metal gases

Molecular Beam Epitaxy (MBE)

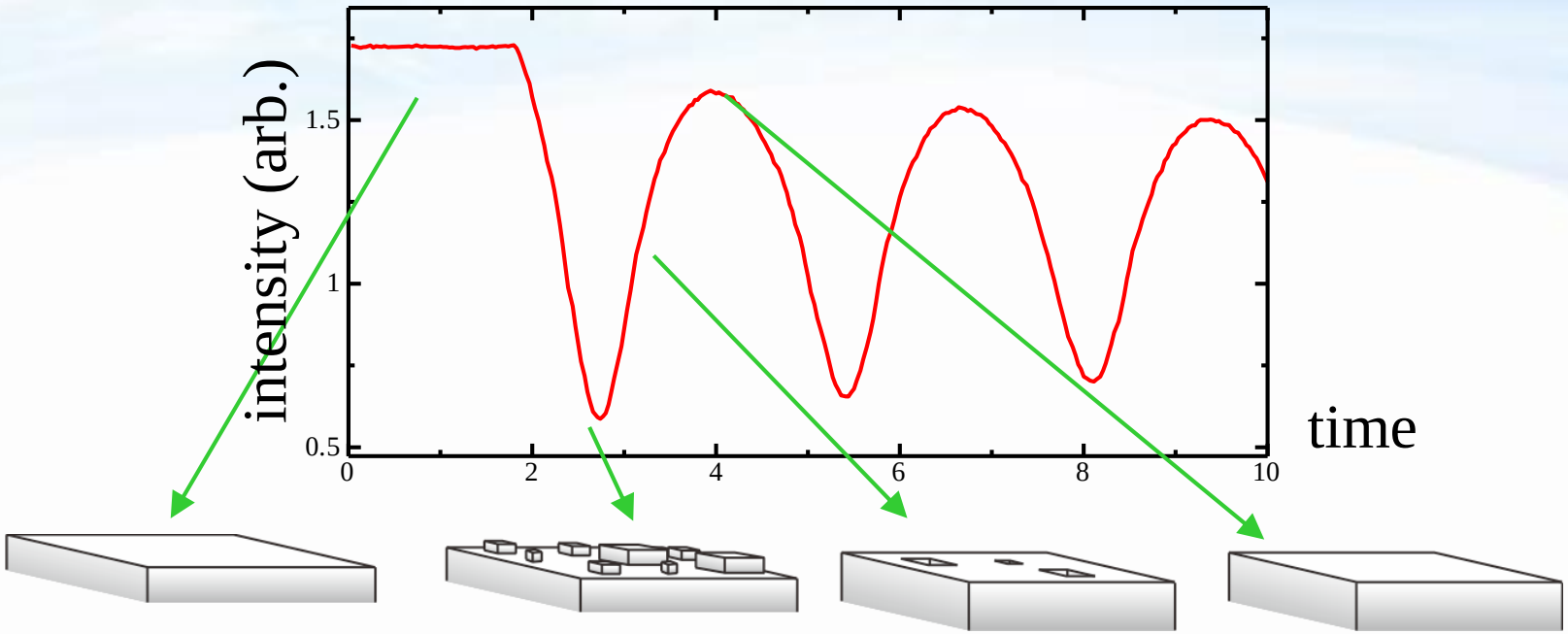
Ultra-high vacuum evaporation



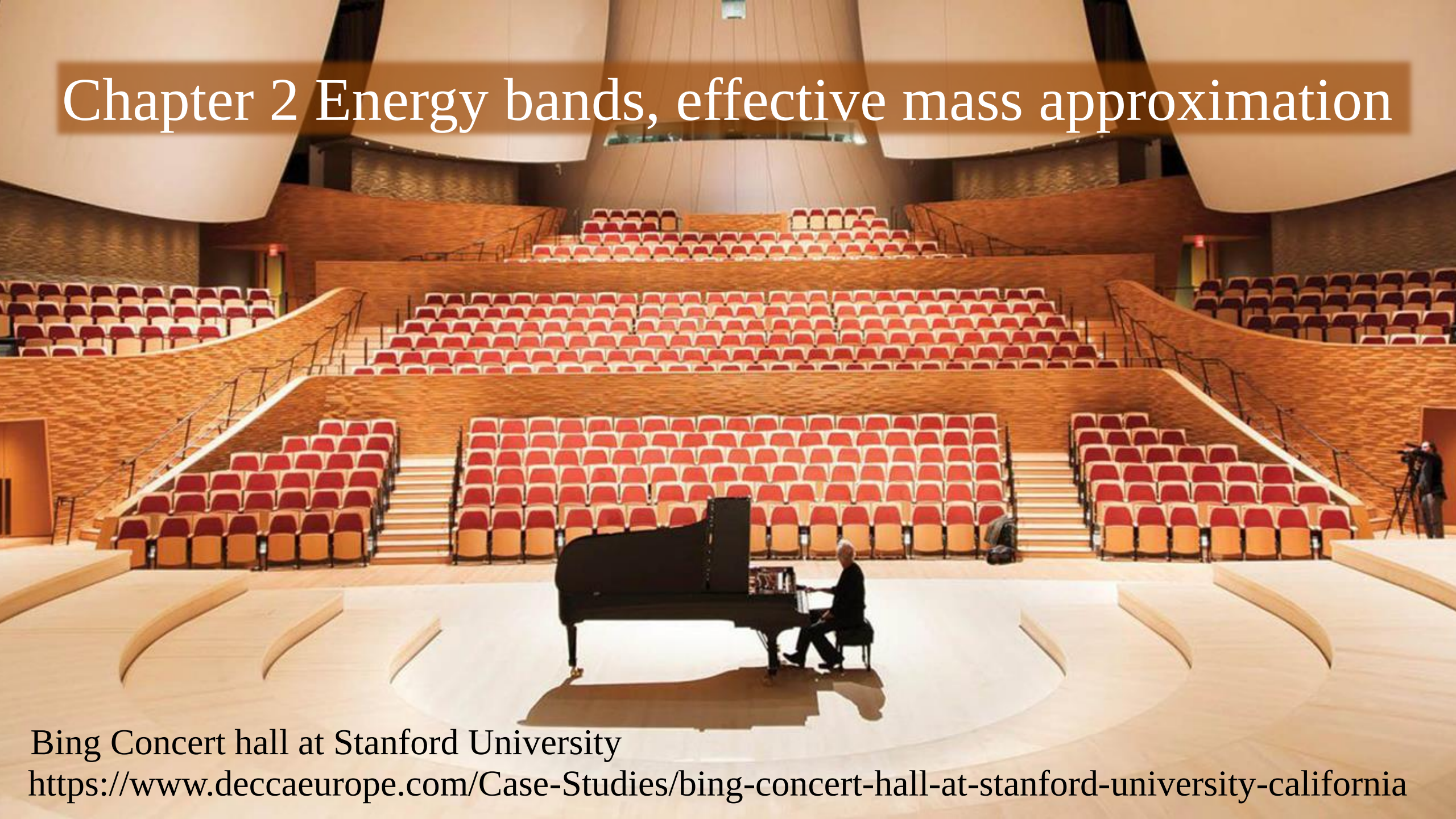
Refractive high energy electron diffraction (RHEED)



HRTEM



Chapter 2 Energy bands, effective mass approximation



Bing Concert hall at Stanford University
https://www.deccaeurope.com/Case-Studies/bing-concert-hall-at-stanford-university-california

Bloch theorem and nearly free electron model

Bloch theorem

Eigenstates in lattice potential:

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r})\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$$

$$u_{n\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{R}) = u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$\boldsymbol{R}$: Lattice translation vector

n: band index

One-dimensional system with a weak periodic potential

$V(x) = 2V_0\cos(k_{\mathrm{w}}x)$ ($k_{\mathrm{w}} = 2\pi/a$, a: lattice const.)

$\langle k'|V|k\rangle = V_0\langle k'|(e^{ik_{\mathrm{w}}x} + e^{-ik_{\mathrm{w}}x})|k\rangle = V_0(\delta_{k'k+k_{\mathrm{w}}} + \delta_{k'k-k_{\mathrm{w}}})$ Perturbation is important from $k \pm k_w$

Energy crossing between $|k\rangle$ and $|k-k_w\rangle$ occurs around $k = k_w/2$

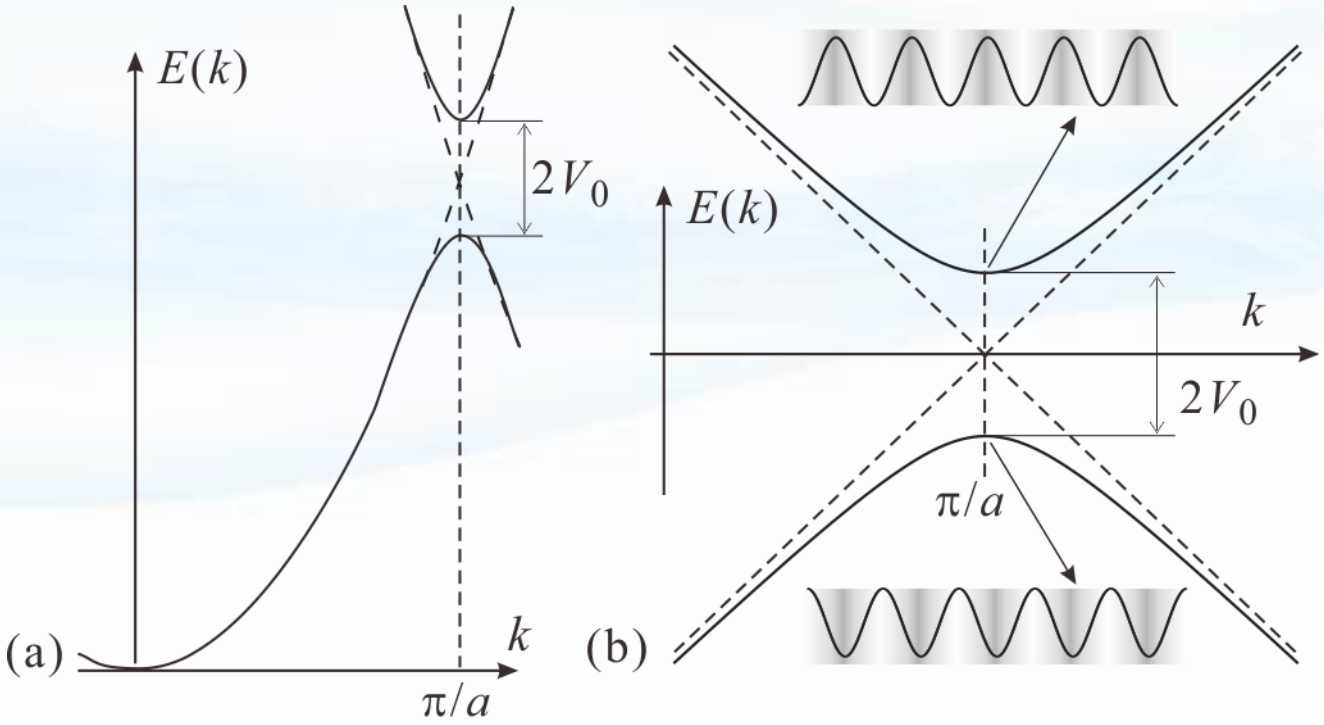
Hamiltonian around $k = k_w/2$ in the space formed with $|k\rangle$ and $|k-k_w\rangle$

$$\mathscr{H} = \begin{bmatrix} \frac{\hbar^2k^2}{2m_0} & V_0 \\ V_0 & \frac{\hbar^2(k-k_{\mathrm{w}})^2}{2m_0} \end{bmatrix} \approx \begin{bmatrix} \epsilon_{\mathrm{z}} - \frac{\hbar^2k_{\mathrm{w}}\Delta k}{2m_0} & V_0 \\ V_0 & \epsilon_{\mathrm{z}} + \frac{\hbar^2k_{\mathrm{w}}\Delta k}{2m_0} \end{bmatrix} \qquad k = k_{\mathrm{w}}/2 - \Delta k$$

Nearly free electron model (2)

$$E_{\pm} = \epsilon_z \pm \sqrt{\epsilon_z \frac{\hbar^2 (\Delta k)^2}{2m_0} + V_0^2} \qquad \epsilon_z = \frac{\hbar^2 k_w^2}{8m_0}$$

Energy gap: $\Delta k = 0 \rightarrow 2V_0$



Overall dispersion

Energy gap due to the phases of standing waves

Bloch theorem

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = u_{n\boldsymbol{k}}(\boldsymbol{r}) \exp(i\boldsymbol{k} \cdot \boldsymbol{r})$$

Standing wave

$$e^{ik_w x/2} \pm e^{-ik_w x/2} = (1 \pm e^{-k_w x}) e^{ik_w x/2}$$
$$= (e^{k_w x} \pm 1) e^{-ik_w x/2}$$

Lattice periodic function

Points $k_w/2$ and $-k_w/2$ are equivalent

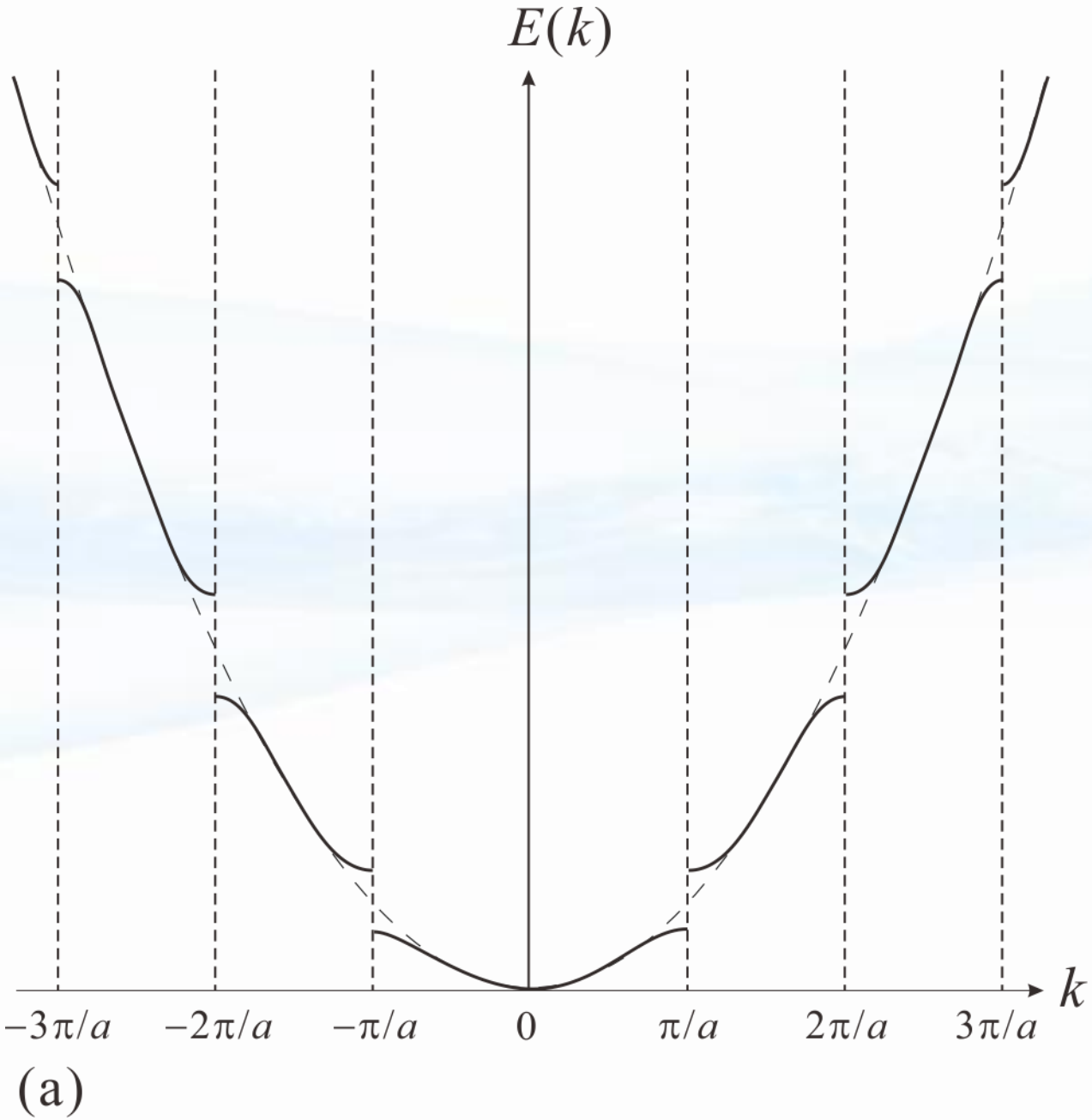
Shifts from these points can be renormalized into $u_{nk}(r)$

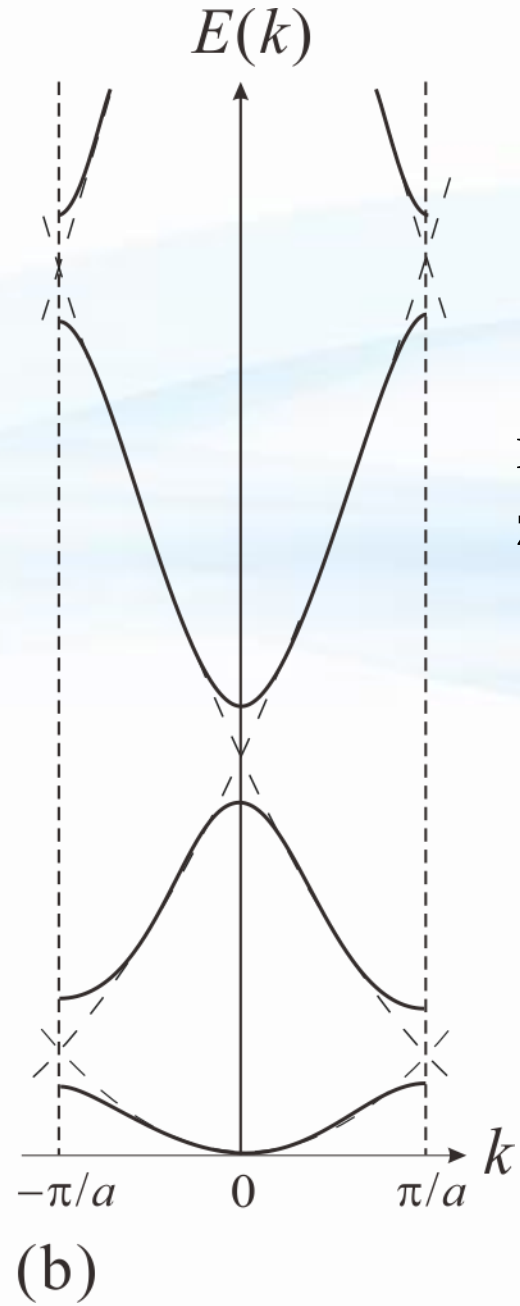
→

Reduced zone expression

Nearly free electron model (3) Reduced zone expression

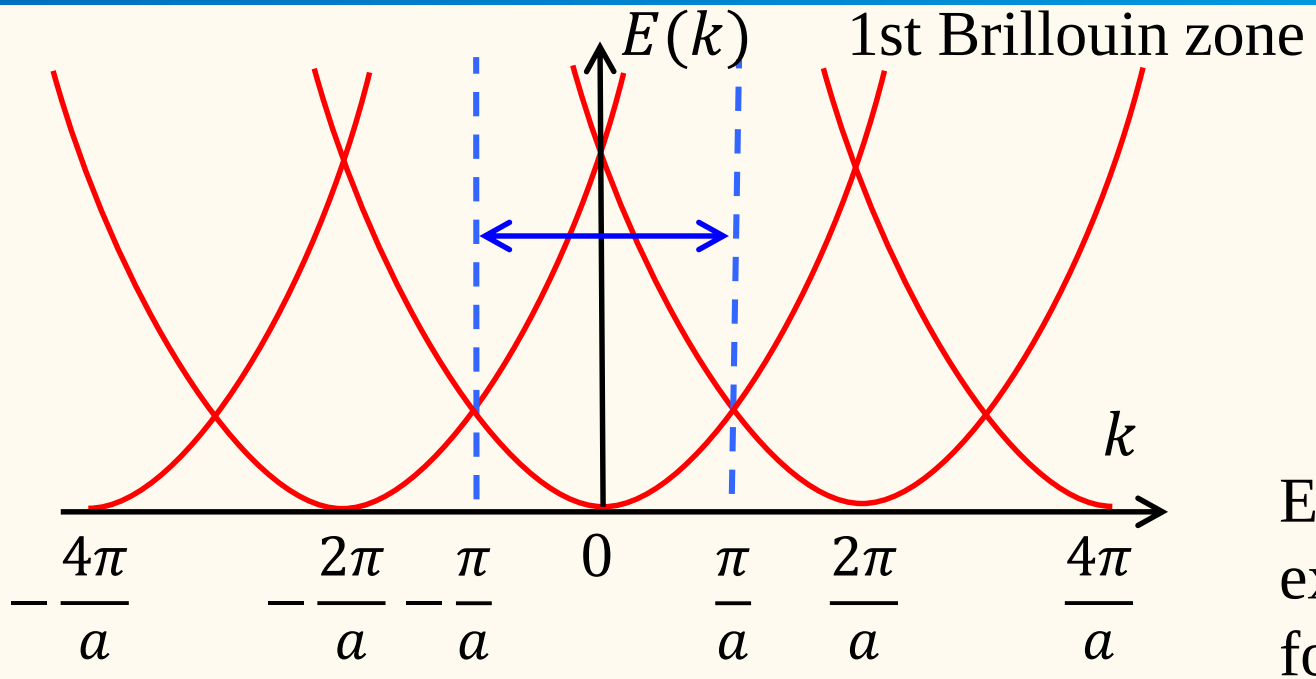
extended zone





reduced zone

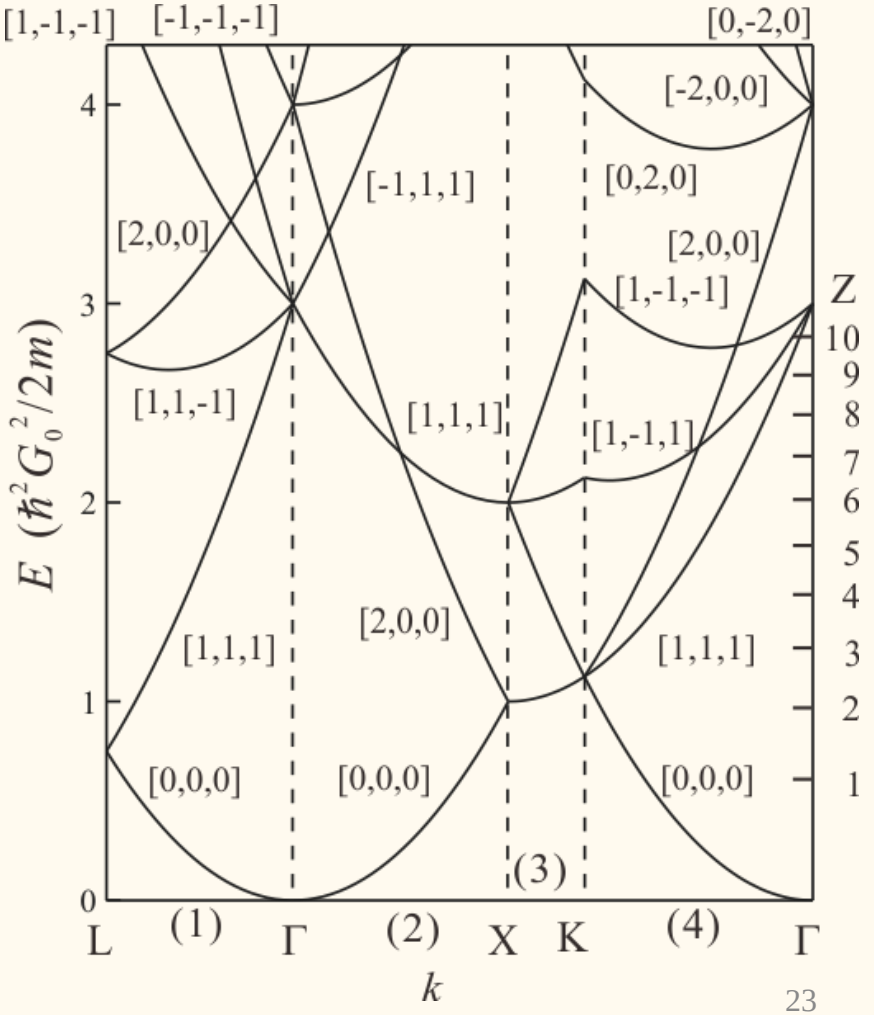
Empty lattice approximation



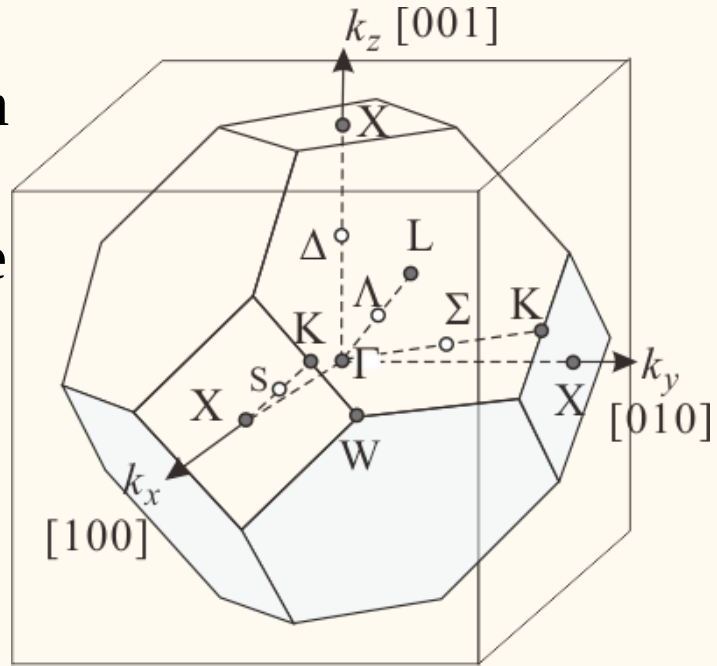
$V_0 \to 0 \qquad e^{ikx} = e^{i(k-k_w)x} e^{ik_w x}$

The free space has a lattice periodicity.

Empty lattice expression for fcc

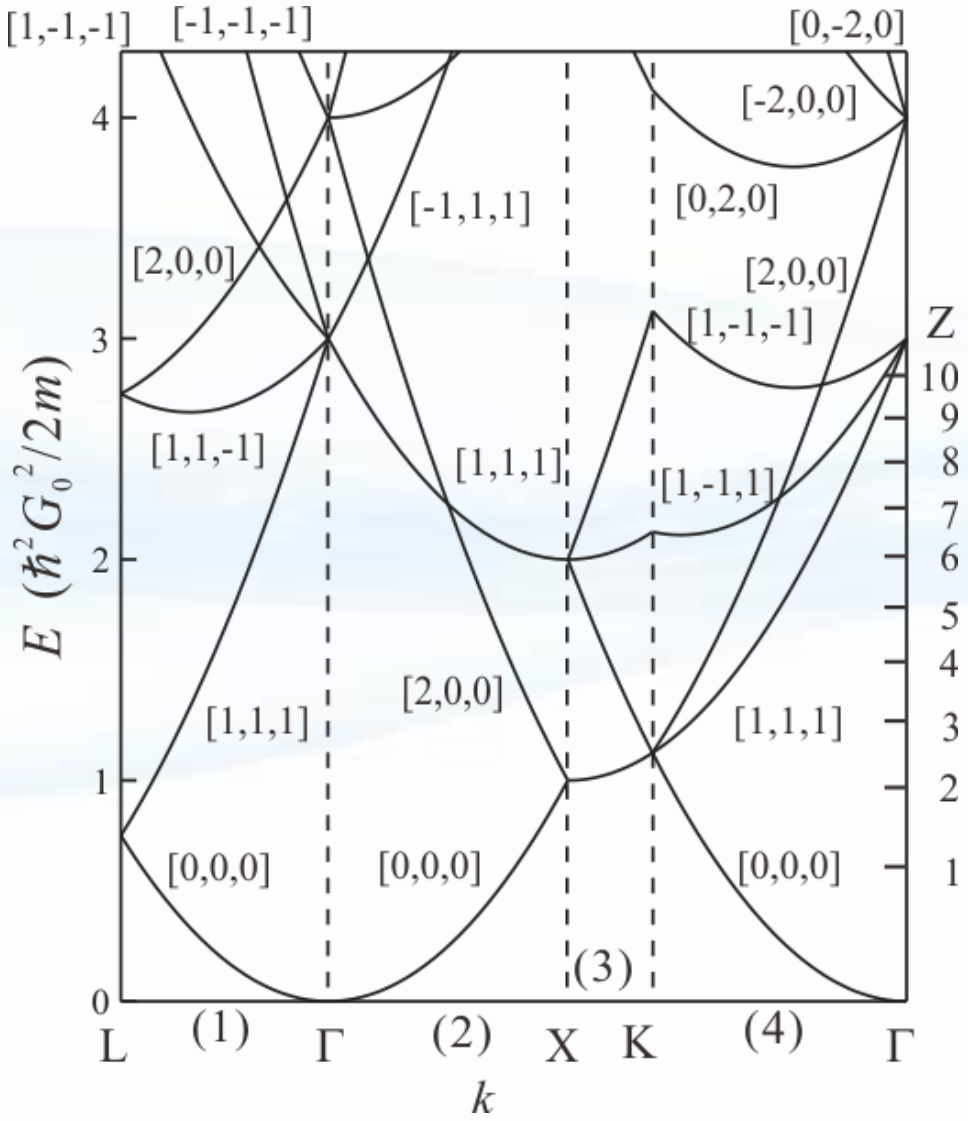


1st Brillouin zone of fcc lattice

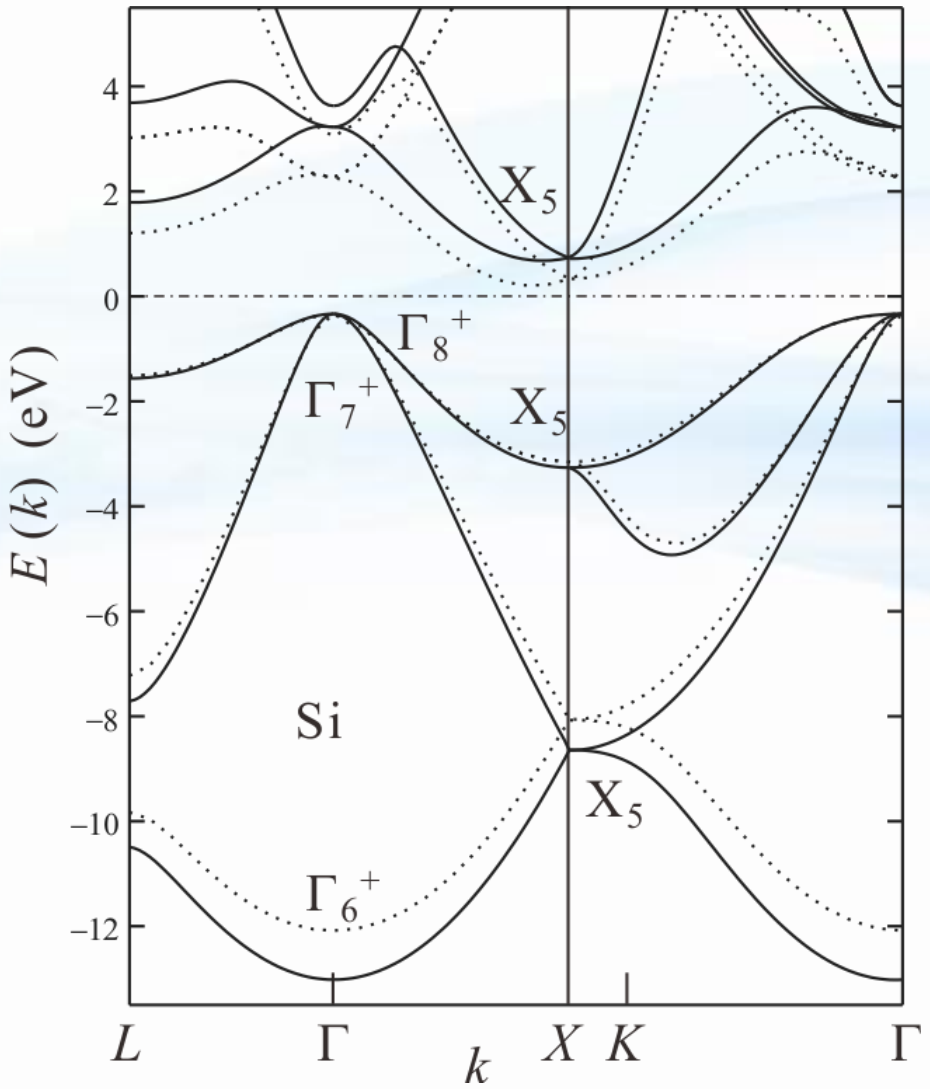


distance	Points	number
0	(0,0,0)	1
$\sqrt{3}$	(1,1,1),…	8
2	(2,0,0),…	6
$\sqrt{8}$	(2,0,2),…	12
$\sqrt{11}$	(3,1,1),…	24

Empty lattice approximation and more realistic band structure



Empty



Si pseudo potential calculation

Tight-binding approximation

Single atom on single unit cell

Single atom Hamiltonian: $\mathscr{H}_a = \hat{T} + u$

$\hat{T}$: kinetic energy, u: atomic potential

$$\mathscr{H}_a(R_i) = \hat{T} + u(r - R_i)$$

$$\mathscr{H}_a(R_i)\phi_n(r - R_i) = \epsilon_n \phi_n(r - R_i)$$

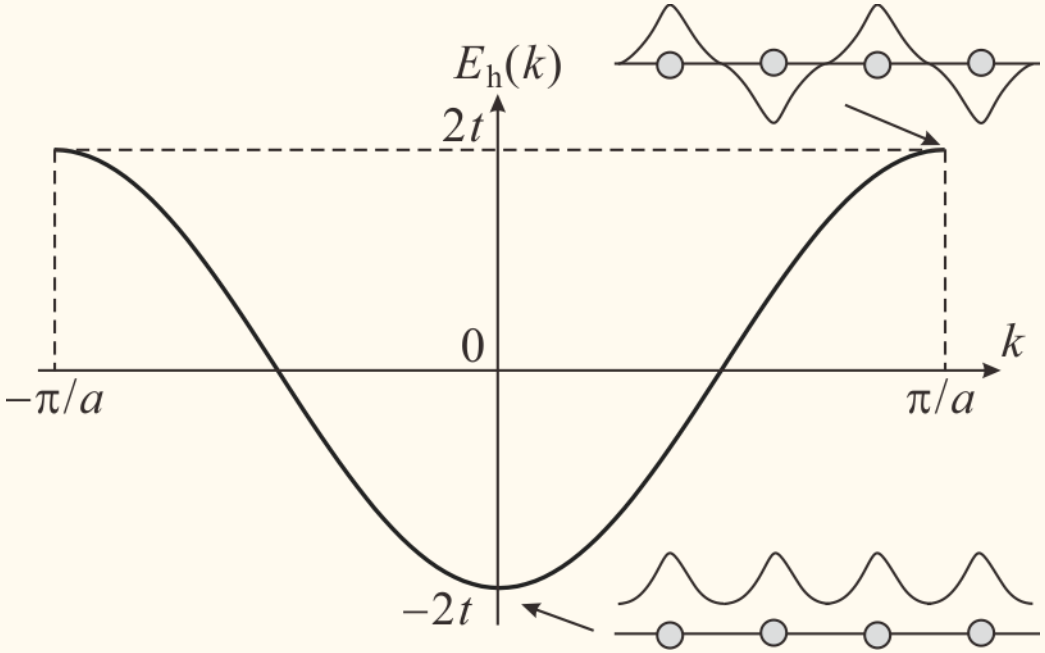
ϕ_n: eigenfunctions for $R_i = 0$

$$\psi_{nk}(r) = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} \phi_n(r - R_i)$$

$$= \frac{e^{ikr}}{\sqrt{N}} \left[\sum_i e^{-ik(r-R_i)} \phi_n(r - R_i) \right]$$

Lattice periodic function

: Bloch form



$$\mathscr{H} = [\hat{T}_x + V(x)]\psi(x) = E\psi(x)$$

Tight binding approximation (2)

$$\langle\psi_{nk}|\mathscr{H}|\psi_{nk}\rangle = N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\langle\phi_n(r-R_i)|[\hat{T}_r+V(r)]|\phi_n(r-R_j)\rangle$$

$$= N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}$$

$$\times\langle\phi_n(r-R_i)|[\hat{T}_r+u(r-R_i)+V(r)-u(r-R_i)]|\phi_n(r-R_j)\rangle$$

$$= \epsilon_n + N^{-1}\sum_{i,j} e^{ik(R_j-R_i)}\langle\phi_n(r-R_i)|[V(r)-u(r-R_i))]|\phi_n(r-R_j)\rangle$$

$$= \epsilon_n + \sum_{j} e^{ikR_j}\langle\phi_n(r)|[V(r)-u(r))]|\phi_n(r-R_j)\rangle.$$

$$E_n(k) = \epsilon_n + \langle\phi_n(r)|v(r)|\phi_n(r)\rangle - \sum_{R_j\neq 0} e^{ikR_j}t_n(R_j)$$

$\alpha_n \equiv -\langle\phi_n(r)|v(r)|\phi_n(r)\rangle$ Crystal field contribution

$t_n(R_j) \equiv -\langle\phi_n(r)|v(r)|\phi_n(r-R_j)\rangle$ Hopping integral

Tight binding approximation (3)

t_n nearest neighbor only = t

$$E_n(k) = \epsilon_n - \alpha_n - t(e^{ika} + e^{-ika})$$
$$= \epsilon_n - \alpha_n - 2t\cos ka$$

Cosine band with the width of $4t$.